

# Induced quantum dots and wires: electron storage and delivery

S. Bednarek, B. Szafran, R.J. Dudek, and K. Lis

*Faculty of Physics and Applied Computer Science,  
AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland*

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We show that quantum dots and quantum wires are formed underneath metal electrodes deposited on a planar semiconductor heterostructure containing a quantum well. The confinement is due to the self-focusing mechanism of an electron wave packet interacting with the charge induced on the metal surface. Induced quantum wires guide the transfer of electrons along metal paths and induced quantum dots store the electrons in specific locations of the nanostructure. Induced dots and wires can be useful for devices operating on the electron spin.

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Planar nanodevices containing single [1, 2, 3, 4, 5, 6], double [7, 8, 9, 10], and multiple [11, 12] laterally coupled quantum dots with confinement potential tuned by electrodes deposited on top of the semiconductor heterostructure are at present extensively studied in both theory and experiment in context of application for quantum gates using electron spins as quantum bits. Recent advances include demonstration that the electron spin can be set and read-out [2, 4, 5, 6, 7, 8, 9, 13] as well as rotated [6, 13]. In a quantum gate working on the electron spins [14] the single qubit operations are to be performed with an electron transfer to a high  $g$  factor region or to a ferromagnetic quantum dot where the electron spin is rotated by microwave radiation. In this letter we present an idea for the control of the electron localization and its transfer between specific locations within the nanodevice. The idea is based on the self-focusing mechanism of an electron wave packet near a conductor surface [15, 16, 17] which as we show below allows to exclude scattering during the electron transfer and warrants the electron delivery to a specific location in the device with a 100% probability.

In the conventional planar nanodevices [1, 2] a negative potential is applied to the gate electrodes to deplete the two-dimensional electron gas underneath. In the variant of the structure proposed below the role of the electrodes is different: a single quantum-well-confined electron becomes self-trapped below the conductor by the potential of the charge that it induces on the metal surface. The response potential of the electron gas of the conductor contains a component of lateral confinement which localizes the quantum-well-confined electron in form of a wave packet that moves parallel to the metal preserving its shape as an electron soliton [15, 16]. The packet was called [17] an *inducton* since the focusing potential stems from the charge induced in the electron gas. The inducton possesses mixed quantum and classical properties. It is described by a wave function of both spatial and spin coordinates whose time evolution is described by the Schroedinger equation. On the other hand the inducton moves as a stable wave packet of a finite size and

its transition probability in transport through potential barriers is binary (0 or 1) [16].

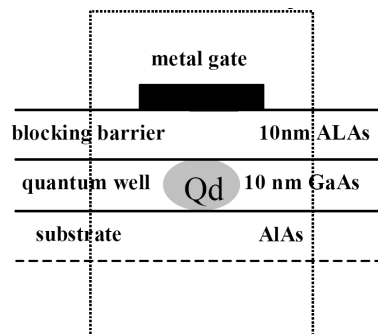


FIG. 1: Cross section of a nanodevice generating an induced quantum dot or wire. Dotted line shows the boundaries of the computational box.

In Ref. [16] we discussed a structure of planar infinite layers of metal, insulator (or semiconducting blocking barrier) and a quantum well in which the inducton was formed. Due to the translational symmetry the inducton can be formed at any place under an infinite metal plate and travel in any direction within the quantum well. In this letter we show that a metal electrode of a finite size is also able to trap an electron underneath it. For the size of the electrode comparable to the inducton radius the transverse motion of the packet is frozen and the induced charge creates a confinement potential similar to the quantum dot potential. A rectangular metal electrode of length larger than the size of the self-focused wave packet leaves the inducton a single degree of freedom for motion along the metal path which therefore forms an induced quantum wire within the quantum well.

The induced potential calculated within the quantum linear response theory is well approximated by the response of an ideal (classical) conductor [16, 17]. Therefore, the induced potential can be quite accurately evaluated by the classical electrodynamics. Let us consider a nanodevice presented in Fig. 1. For an infinite metal plate the induced potential can be evaluated with the im-

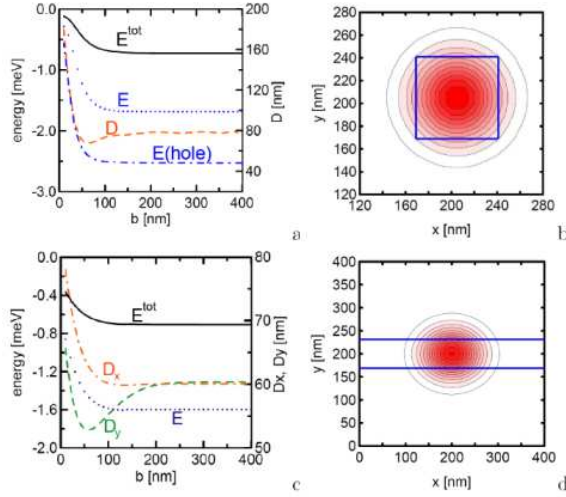


FIG. 2: (a) Total energy  $E^{tot}$ , single electron energy  $E$ , and diameter of the wave packet  $D$  for a quantum dot induced by square metal plate of side length  $b$ . Dash-dotted curve shows the eigenvalue  $E$  for a heavy hole inductor ( $m = 0.45m_0$ ). (b) Electron density in the quantum dot induced by square metal plate with  $b = 70$  nm. (c)  $E^{tot}$ ,  $E$  and packet length along  $x$  and  $y$  direction ( $D_x, D_y$ ) for a quantum wire induced by an infinite metal bar of width  $b$ . (d) Charge density of the wave packet confined under the metal bar of width  $b = 50$  nm.

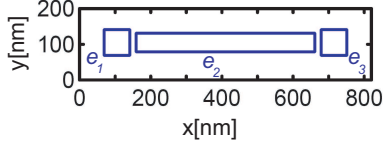


FIG. 3: Top view of the setup to transfer the electron from the quantum dot induced under the electrode  $e_1$  to the quantum dot induced under  $e_3$  via the quantum wire induced under  $e_2$ .

age charge method [16] which greatly simplifies the calculations but is no longer applicable for metal plates of finite size. The induced potential is therefore calculated from the Poisson equation. We apply the theory used previously for the electrostatic quantum dot modeling [18] which describes experiments with remarkable accuracy. The presence of the metal introduces fixed potential value in the boundary conditions at the conducting surface. All the nanodevice is contained in a rectangular computational box (see the dotted line in Fig. 1). We require the normal component of the electric field at the surface of the box to vanish. The size of the box is taken large enough that for an infinite metal plate we reproduce the image charge potential. We solve the Poisson

equation

$$\nabla^2 \Phi(\mathbf{r}) = -\frac{1}{\epsilon\epsilon_0} \rho(\mathbf{r}) \quad (1)$$

where the charge density is expressed by the electron wave function  $\psi(\mathbf{r})$  and the electron charge  $-e$ :

$$\rho(\mathbf{r}) = -e|\psi(\mathbf{r})|^2. \quad (2)$$

According to the superposition principle the calculated total potential  $\Phi$  is a sum of contributions stemming from two sources

$$\Phi(\mathbf{r}) = \phi_1(\mathbf{r}) + \phi_2(\mathbf{r}), \quad (3)$$

where  $\phi_1$  is directly due to the charge density distribution

$$\phi_1(\mathbf{r}) = \frac{-e}{4\pi\epsilon\epsilon_0} \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (4)$$

and the second component is due to the charge induced on the electrode which creates the lateral confinement for the electron localized in the quantum well. Given the total potential  $\Phi$  and the potential of the electron packet  $\phi_1$  the induced potential  $\phi_2$  is calculated according to

$$\phi_2(\mathbf{r}) = \Phi(\mathbf{r}) - \phi_1(\mathbf{r}). \quad (5)$$

For the nanostructure of Fig. 1 the motion of the electron in the growth direction is frozen by the strong vertical confinement which can be eliminated from the Schrodinger equation thus taking a two dimensional form

$$H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - e\phi_2(x, y, z_0), \quad (6)$$

where  $z_0$  is the center of the quantum well. In the eigenequation

$$H\psi = E\psi, \quad (7)$$

$E$  is the single-electron energy [16]. The total energy is obtained [16] by subtracting half of the interaction energy of the inductor with the induced potential:

$$E^{tot} = E + \frac{e}{2} \int dx dy |\psi(x, y)|^2 \phi_2(x, y, z_0). \quad (8)$$

The  $\phi_2$  potential and the wave function  $\psi$  are mutually dependent so the problem is solved in a self-consistent iteration.

Let us assume that the metal electrode deposited on top of the semiconductor (see Fig. 1) is of a square shape with side length  $b$ . We solve equations (1-8) and evaluate the average diameter of the electron wave packet

$$D = 2 \int dx dy \sqrt{(x - x_0)^2 + (y - y_0)^2} |\psi(x, y)|^2, \quad (9)$$

where  $(x_0, y_0)$  are the coordinates of the center of the metal square. GaAs electron effective mass  $m = 0.067m_0$  and dielectric constant  $\epsilon = 12.5$  are adopted.

The single-electron energy, the total energy and the packet diameter are plotted as function of  $b$  in Fig. 2(a). Both the energies are negative (for any  $b$ ) and decrease with growing  $b$  reaching the free inducton (electron wave packet under an infinite metal plate) limit [16]. The limit is obtained for  $b$  larger than the free inducton radius. The packet diameter is a non monotonic function of  $b$ . For small plate the packet is large, localization is the strongest for  $b_{min}^{dot} = 70$  nm and for  $b > b_{min}^{dot}$  the diameter grows to the free inducton limit. Soon after the minimal diameter is reached the energies saturate as function of  $b$ . Note that the minimal diameter is nearly equal to  $b_{min}^{dot}$  (for the charge density and the size of the plate see Fig. 2(b)). The  $b_{min}^{dot}$  value is optimal for the proposed applications of electron storage and transfer (see below).

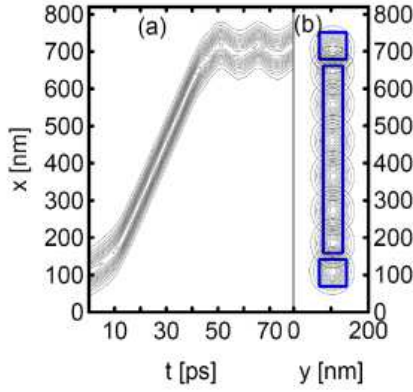


FIG. 4: Time evolution of the electron density in the device with straight path. (a) Electron charge density as function of the  $x$ -variable and time calculated at the symmetry axis of the electrode configuration presented with blue lines in (b). The contour plots in (b) display the charge density at subsequent moments in time.

Similar calculation was performed for the electrode in form of a metal bar that is infinite in the  $x$ -direction and of width  $b$  in the  $y$ -direction (it will be referred to as a current path). Fig. 2(c) shows both the energies and the size of the packet in both directions of the quantum wire

$$D_x = 2 \int dx dy |x - x_0| |\psi(x, y)|^2 \quad (10)$$

$$D_y = 2 \int dx dy |y - y_0| |\psi(x, y)|^2. \quad (11)$$

Quite remarkably values of  $D_x$  and  $D_y$  are close, although only  $D_y$  has a minimum as a function of  $b$ . The strongest focusing appears for the current path of width  $b_{min}^{wire} = 50$  nm, adopted as optimal in the following. The charge distribution for  $b = b_{min}^{wire}$  plotted in Fig. 2(d) shows

that the packet is more strongly localized in the direction perpendicular to the path.

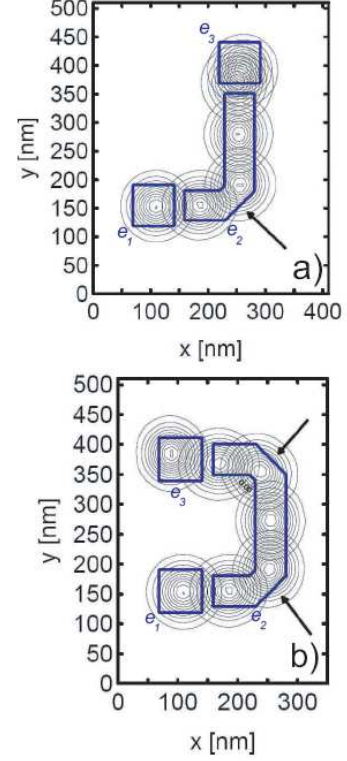


FIG. 5: Snapshots of the time evolution of the electron density following the path broken once (a) or twice (b). The arrows indicate the cut corners of the metal paths. The electron leaves the quantum dot induced under the  $e_1$  electrode and goes to the quantum dot under  $e_3$ .

In the calculations discussed above the stationary eigenproblem (7) of Hamiltonian (6) was solved by the evolution in the imaginary time [19] which leads to formation of the ground state wave function. A slight modification of the approach allows to investigate the evolution in the real time. For that purpose the time dependent Schroedinger equation is solved:

$$d\psi(\mathbf{r}, t) = \frac{i}{\hbar} H(\mathbf{r}, t) \psi(\mathbf{r}, t) dt. \quad (12)$$

The dependence of the Hamiltonian on time appears for a moving inducton due to the time dependence of the electron density which enters Eqs. (1) and (4)

$$\rho(\mathbf{r}, t) = -e |\psi(\mathbf{r}, t)|^2. \quad (13)$$

The time dependence of the potential is accounted for by solving Eqs. (1,4,5) for each time step (12).

Let us consider a nanodevice whose cross section agrees with the schematic of Fig. 1 and the top view is displayed in Fig. 3. On the surface of the structure we have three electrodes separated by gaps of 20 nm. Quantum dots are

formed below square electrodes  $e_1$  and  $e_3$  both of size  $70 \text{ nm} \times 70 \text{ nm}$ . The middle electrode  $e_2$  ( $50 \text{ nm} \times 500 \text{ nm}$ ) is supposed to induce a quantum wire which should guide an electron from under  $e_1$  to  $e_3$ .

We assume that the electron is confined below  $e_1$  for a time long enough to relax to the ground state. In the simulation it is achieved by the imaginary time evolution for potentials of the electrodes (the Schottky barrier neglected):  $V_1 = 0.0 \text{ mV}$ ,  $V_2 = V_3 = -0.1 \text{ mV}$  ( $V_1, V_2, V_3$  are the potentials applied to  $e_1, e_2, e_3$  electrodes respectively). After the induction relaxes to the ground state we change the applied voltages putting  $V_1 = -0.1 \text{ mV}$ ,  $V_2 = 0.0 \text{ mV}$ ,  $V_3 = -0.1 \text{ mV}$  and we start the evolution in the real time. The inversed  $V_1 - V_2$  potential difference gently sets the electron in motion. The electron gains the kinetic energy passing from below  $e_1$  to  $e_2$ . Next it goes along  $e_2$  with a constant kinetic energy eventually reaching the quantum dot induced under  $e_3$ . At that moment  $V_2$  voltage is switched to  $V_2 = -0.15 \text{ mV}$  to confine the electron permanently under  $e_3$ . The traveling electron density is presented in Fig. 4(b) for several moments in time. In Fig. 4(a)  $|\psi(x, y_0, t)|^2$  is plotted for  $y_0 = 200 \text{ nm}$  set at the symmetry axis of the proposed setup. We can see that the induction is accelerated between  $e_1$  and  $e_2$  (see the curved shape of the density plot in Fig. 4(a) between  $x = 100$  and  $200 \text{ nm}$ ). Then it moves with a constant velocity under  $e_2$  [note increased localization of the packet when under  $e_2$ ]. Finally the packet gets under  $e_3$  and is trapped there when  $V_2$  is switched to negative. The oscillations observed in Fig. 4 (a) for  $t > 50 \text{ ps}$  are due to the residual kinetic energy which is not lost when the induction is trapped under  $e_3$ . The crucial point of the presented results is that the electron was transferred from one dot to the other with a 100 % probability which is due to the self-focusing mechanism.

Let us consider a similar structures but with varied shape of the electrodes (blue lines in Fig. 5(a) and Fig. 5(b)). The middle electrode turns under right angles to force the induction to change direction of its velocity vector. The time evolution is presented in Fig. 5. It turns out that the electron can be guided under any place in the structure also along curved paths. Note the cut corner edges of the current path marked in Fig. 5 with arrows. It allows the electron to change the motion direction with equal incident and reflection angles. For an uncut edge with a  $90^\circ$  angle the electron is reflected back to  $e_1$ .

The  $b_{min}$  values adopted above for the size of the electrodes are optimal for three reasons: 1) the confinement in quantum dots is the strongest 2) the motion along the wires follows the axis of the wire most closely 3) the electron still penetrates the region that is not covered by the electrode that induces the confinement [see Figs. 2(c) and (d)] and can therefore be set in motion by voltage applied to adjacent electrodes.

To conclude, we presented a design for a planar semiconductor structure with a quantum well and electrodes separated by a tunnel barrier in which induced quantum dots and quantum wires are formed. The dots store the electrons in specific points of the nanostructure and the paths assist in the transport of the electrons between chosen locations in the device. The self-focusing effect allows the electron to be kept in the stable wave packet (induction state) of a size close to the electrode width. It also allows the electron transport with a 100% probability of passing through obstacles in form of potential cavities or barriers. The combination of semi-classical transport properties of the induction with its spin degree of freedom is likely to become useful for the spin operating devices. The induction binding energy is not large (of order of  $1.5 \text{ meV}$ ), but this is enough for the wave packet to overcome the potential barriers on its way under the metal paths [20].

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  - [20] The binding energy of a hole induction with  $m = 0.45m_0$  (see the dash-dotted line in Fig. 2(a)) is by about  $1 \text{ meV}$  stronger since the larger mass allows for stronger localization which enhances the electron-metal interaction energy.